

COURSE SYLLABUS

1. COURSE DESCRIPTION

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| Degree: | Biología |
| Double Degree: | |
| Course: | Chemical Thermodynamics and Kinetics |
| Module: | BLOQUE 1 MATERIAS BÁSICAS |
| Department: | Sistemas Físicos, Químicos y Naturales |
| Academic Year: | 2013-14 |
| Term: | First Term |
| Total Credits : | 6 |
| Year: | 1 |
| Type of Course: | Basic |
| Course Language: | English |

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| Modelo de docencia: | B1 |
| a. Enseñanzas Básicas (EB): | 60% |
| b. Enseñanzas de Prácticas y Desarrollo (EPD): | 40% |
| c. Actividades Dirigidas (AD): | |
| d. | |

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2. TEACHING TEAM INFORMATION

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| Course Coordinator: Patrick Merkling | |
| Professors | |
| Name: | Dr. Juan Antonio Anta |
| Faculty: | Facultad de Ciencias Experimentales |
| Department: | Sistemas Físicos, Químicos y Naturales |
| Academic Area: | Química Física |
| Category: | Prof. Titular |
| Office Hours: | TBD and by appointment (e-mail me to arrange a time) |
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| | |
| Name: | Dr. Reyes de la Vega |
| Faculty: | Facultad de Ciencias Experimentales |
| Department: | Sistemas Físicos, Químicos y Naturales |
| Academic Area: | Química Física |
| Category: | Prof. Asociado |
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3. ACADEMIC CONTEXT

3.1. Course Description and Objectives

Biotechnology deals with the use of living organisms or chemicals of biological origin to obtain products which involve an economical, health or social added value. For this reason, learning Biotechnology at an undergraduate degree level brings about acquiring basic knowledge in Chemistry and Biology, so that students can understand technological processes which are used in living organisms.

3.2. Contribution to the training plan

The assignment of Chemical Thermodynamics and Kinetics belongs to the module “Chemistry in Molecular Biosciences”. Within this module, the General Chemistry Course provides the students with the fundamentals and capabilities needed to understand the mechanisms underlying biological processes.

The general and specific skills achieved in this course are essential to understand further advanced matters that they will study in their degree, such as Instrumental Analysis Techniques, Bioanalytical Chemistry, Biochemistry, etc.

3.3. Recommendations or prerequisites

Recommendation: having studied chemistry, physics and maths

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4. SKILLS

4.1 Degree skills developed during this course

Biotechnology can be defined as a technique that uses living organisms or compounds obtained from living organisms to produce products of economical, medical or social value to humans. Therefore learning about Biotechnology at the level of the Degree requires a biological and chemical knowledge base to enable students to understand the technological processes that involve living organisms.

The Report for the verification request of the graduate degree in Biotechnology from the University Pablo de Olavide referred (among others) the following competencies:

- Understand the scientific method. Know, understand and apply the tools, techniques and experimental protocols in the laboratory and acquire the skills of observation and interpretation of the results.
- Acquire basic experimental skills appropriate to each of the subjects taught, by the description, quantification, analysis and critical evaluation of the experimental results obtained independently.
- Work properly in a biological, chemical or biochemical laboratory, know and apply standards and techniques related to health and safety, handling of laboratory animals and waste management.
- Demonstrate proper integrated view of the R + D + i be able to interrelate and connect the areas of biotechnology encompassing knowledge from biological and physicochemical principles to new scientific knowledge for practical application development and introduction in the market for new biotech products of interest

4.2. Module skills developed during this course

The Degree Report includes the following module-specific skills:

1. Know the origin of the atomic/molecular properties of matter, including pure substances, mixtures and solutions.
2. Know the principles of thermodynamics and their practical application to thermochemical and thermodynamic study of a reaction and dominate the thermodynamic concept of chemical equilibrium and equilibrium constant, and be able to identify the factors on which it depends.
3. Learn the common characteristics of physicochemical transport processes: diffusion, osmosis, electrophoresis, etc ...
4. Master the concept of reaction rate and rate constant and be able to identify the factors on which it depends and know how to describe proton transfer reactions and electronical and thermodynamical concepts applied to their behavior.
5. Know the basis of spectroscopical methods for quantitative chemical analysis and structural elucidation of organic compounds.



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4.3. Course-specific skills

1. Understand the atomic/molecular origin of the properties of matter, either pure substances, mixtures or solutions
2. Apply the principles of thermodynamics to thermochemical and thermodynamic study of a chemical reaction
3. Master the concept of chemical equilibrium and equilibrium constant, and be able to identify the factors on which it depends
4. Master the concept of reaction rate and rate constant and be able to identify the factors on which it depends
5. Be able to describe the proton transfer reactions and electronic and thermodynamic concepts involved in their description

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5. COURSE CONTENTS (COURSE TOPICS)

In order to accomplish the aforementioned goals, the contents of this course are distributed in 10 Units, as described in the table below. Each Unit has a number of EB and EPD hours which depend on their relative importance for the learning of Chemical Kinetics and Thermodynamics for Biotechnology students. There will be four 3-hour laboratory exercises and three slots of 2-hour seminars.

Part A: Introduction and Chemical Thermodynamics

| | Contents | Hours EB | Hours EPD |
|---|---|-------------|---|
| Unit 1: Introduction | <i>Course organization and general concepts</i> | 1 | |
| Unit 2: Basic definitions and the First Law | <i>Concept of "system" and "variable" in Thermodynamics. Thermodynamic Equilibrium. Response functions. Equations of State: The ideal gas equation and the virial equation. Heat and Work. Mechanical Work, electric Work, surface Work and chemical Work. Equivalence between Heat and Work. Internal energy and the First Law. Enthalpy. Thermochemistry and Hess Law.</i> | 3 | Seminar <i>Solving Exercises</i> <i>Units 2 and</i> <i>(2 hours)</i> |
| Unit 3: The Second and the Third Laws | <i>Spontaneity and directionality of the physicochemical processes. Entropy and the Second Law. Fundamental Equation of Thermodynamics. The concept of Thermodynamic Potential and Free Energy. Calculations involving variables and thermodynamic derivatives. The Third Law and Absolute Entropies. The Microscopic Basis of Thermodynamics: an introduction to Statistical Thermodynamics.</i> | 4 | |
| Unit 4: Phase Equilibria | <i>Mass as a thermodynamic variable. Chemical Potential. Gibbs-Duhem equation. The relationship between activity and chemical potential. Reference states. Phase transitions and Phase Diagrams in pure substances. Clapeyron and Clausius-Clapeyron Equations. Phase diagrams for binary mixtures. Raoult's Law and Henry's Law. Colligative properties.</i> | 3 | Laboratory Exercise Determination partition coefficient Acetic Acid water/organic (3 hours) |

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| Unit 5: Chemical Equilibrium | <i>Determination of the reaction free energy. Thermodynamic Description of Chemical Equilibrium. Definition of Equilibrium Constant. Factors affecting the Chemical Equilibrium: composition and temperature. Van't Hoff's Law.</i> | 3 | Seminar <i>Solving Exercises</i> <i>Units 4 and</i> <i>(2 hours)</i> |
| | TOTAL | 14 | 7 |

Part B: Kinetics and Complex Systems

| | Contents | Horas EB | Horas EPD |
|--|--|-------------|---|
| Unit 6: Transport processes | <i>Introduction of the time variable in physicochemical processes. Concept of thermodynamic gradient and flux. Continuity equation. Diffusion, viscosity, thermal conductivity and electrical conductivity. Fick's Laws. Equations of Stokes-Einstein and Einstein-Smoluchowski.</i> | 3 | |
| Unit 7: Formal Chemical Kinetics | <i>Concept of reaction rate. Rate equation and reaction orders. Integrated rate equation. First order and Second order chemical reactions. Concept of lifetime.</i> | 2 | |
| Unit 8: Molecular Chemical Kinetics | <i>Concept of molecularity and reaction mechanism. Concept of steady state and rate-limiting step. Temperature effect and Arrhenius Equation. Catalysis. Types of Catalysis: homogenous, heterogenous and enzymatic. Michaelis-Menten mechanism.</i> | 3 | |
| Unit 9: Thermodynamic of electrolytic solutions and electron-transfer reactions. | <i>Ions in solution. Debye-Hückel law. Relationship between free energy and electric potential. Ion transport and electrochemical potential. Membrane potential. Electron-transfer chemical reactions: Nernst equation</i> | 3 | |
| Unit10: Colloidal systems and colloidal stability | <i>Concept of colloidal system. Types of colloidal systems. Stability and aggregation of macromolecules and colloids.</i> | 2 | Práctica <i>Measurement</i> <i>Isoelectric</i> <i>Casein.</i> <i>(3 hours)</i> |
| | TOTAL | 13 | 11 |



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6. METHODOLOGY AND RESOURCES

Classes are of two general types "basic teaching" (EB) and "practices and development" (EPD). The EPD in this course are either 3-hour lab sessions or 2-hour seminars. For more details a table in the expanded teaching guide will be made available through the virtual platform.

Methodologically, transparencies will be used, seminars, individual tutorials, laboratory, and, if technology permits, use of the virtual platform.

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7. ASSESSMENT

This course devotes 15 hours for evaluation. This is organized as follows:

- e. Final EB exam: 3 hours (February)
- f. Final EPD-laboratory: exam 45 minutes (February)
- g. Final EB exam (retake): 3 hours (July)
- h. Final EPD-laboratory exam (retake): 45 minutes (February)
- i. Seminar hand-outs: 6 hours (one hand-out per seminar)
- j. Poster session: 1.5 horas.

The students should bear in mind the following issues:

- a. The **Final EB exam** will be composed of 3 or 4 numerical problems from Parts A and B.
- b. The **Final EPD-laboratory exam** will be composed of one question for each of the practical exercise done in the laboratory. The students may bring their laboratory notes to the exam to help them answer the questions. It is then important to carry out the laboratory exercises properly and correctly annotate the main results and conclusions.
- c. To evaluate the **seminars**, a list of 4-5 problems will be proposed for each seminar. The problems will be submitted by the students in legible handwriting before the seminar, and then solved and discussed by the teacher during the seminar. During the following week a 30-minutes exam will be held, where each student will have to solve one the proposed problems individually. The seminar mark will be calculated from the problems submission (25%) and the individual exam (75%). Tutorials for the seminars are only allowed via the virtual platform.
- d. At the end of the semester, a 2-hours **poster session** will be held, where groups of 3-4 students will give a presentation, in the form of a poster, on one of the following topics: Enzymatic Kinetics, Biomolecules, Interfases, Colloidal Systems, or related. The poster mark will be calculated from the teacher's marks (50%) and from the students themselves (50%). An article to be published in the Moleqla journal (www.upo.es/moleqla/) would be optionally accepted after the poster session.

The final mark of the course will be extracted from the following mathematical formula:



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$$\text{MARK} = 0.6 \times \text{Final EB} + 0.15 \times \text{Seminar Problems} + 0.15 \times \text{Final EPD-laboratory} + 0.1 \times \text{Poster-session}$$

To pass the course, a minimum of 5 points out of 10 will be required, provided a minimum of 4.5 points in the Final Exam EB is achieved. This means that realization of the EB Final Exam is mandatory to pass the course, whereas the rest of the elements in the evaluation are facultative. Furthermore, 6 points minimum in the EB Final Exam are required for “Remarkable” mark (“Notable”). Attendance to the lab sessions is mandatory.

Once the retake exams for both EB and EPD-lab (July call) are held, the marks obtained from the Seminar Problems and the Poster-session during the normal teaching period will be kept and considered to calculate the final mark of the course. However, upon student request, an special exam covering a 100% of the total mark of the course can be prepared. This exam will include the examination of all skills taught during the course. In case the student does not pass the course, partial marks (EPD, Seminars, etc.) are not kept for subsequent years.

8. BIBLIOGRAPHY

(Those in the UPO library are marked with *)

EB

- a. *Curso de Termodinámica** A. Peris, Alhambra Universidad (2006)
- b. *Fisicoquímica**, P.W. Atkins y J. De Paula, 4th Edition, Oxford University Press (2003)
- c. *Termodinámica (I y II)**, Y.A. Çengel y M.A. Boles, Ed. McGraw Hill, 2001
- d. *Termodinámica**, Kenneth Wark, McGraw-Hill, D. L. 2003
- e. *Calor y termodinámica*, M.W. Zemansky y R.H. Dittman, Ed. McGraw-Hill, 1990.
- f. *Termodinámica Química y de los procesos irreversibles**, Criado Sancho, Manuel Madrid [etc.] : Pearson Educación : Addison Wesley, 2004
- g. *Termodinámica Química**, J. Rodríguez-Renuncio, Editorial Síntesis (2000)

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- h. *Fundamentos de Cinética Química**, S. R. Logan, Addison Wesley Publishing Company (2000).
- i. *Cinética Química para Sistemas Homogéneos (libro electrónico)**, Jorge **Ancheyta Juárez, Miguel ángel Valenzuela Zapata**. Publicación México : Instituto Politécnico Nacional, 2002.
- j. *The elements of Physical Chemistry**, P. Atkins, Oxford : Oxford University Press, 2001
- k. *Physical chemistry for the Life Sciences**, P.W. Atkins y J. De Paula, Oxford : Oxford University Press, cop. 2006
- l. *Physical chemistry for the Biological Sciences**, Gordon **G. Hammes** Publicación Hoboken, NJ : John Wiley, cop. 2007
- m. *Physical Chemistry. Principles and Applications in Biological Sciences*, Tinoco-Sauer Wang-Puglisi, 4th Edition, Prentice-Hall (2002)
- n. *Molecular Driving Forces.** Ken a Dill y Sarina Bromberg. Garland Science

Problems

- a. *Problemas resueltos de termodinámica**, María del Barrio Casado, Eduardo Bravo Guil, Francisco J. Lana, Pons, David O Pérez, Perez, et al. (Parainfo), ISBN: 8497323491. ISBN-13: 9788497323499, 2005
- b. *Termodinámica: 100 problemas y ejercicios resueltos**, Hubert Lumbroso, Barcelona Reverté, D.L. 2005
- c. *100 problemas de termodinámica**, Julio Pellicer y José Antonio Manzanares. Alianza Editorial, 1996
- d. *Teoría y problemas de termodinámica*, M. M. Abbot, H. C. van Ness. McGraw-Hill, 1990.
- e. *Problemas de termodinámica**, J.M. Lacalle, R. Nieto, M.C.Gonzalez. E.T..S. de Ingenieros Industriales, Universidad Politécnica de Madrid, 1993
- f. *Termodinámica: 100 ejercicios y problemas resueltos*, Hubert Lumbroso. Ed. Reverté, 1979
- g. *Problemas de termodinámica y mecánica estadística*, J. Aguilar Peris, J. de la Rubia Pacheco, C. Fernandez Pineda. Ed. Saber, 1971
- h. *Problemas programados de termodinámica**, E.Braun, E.T. Wait. Ed. Reverté, 1973



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- i. *Teoría y problemas de termodinámica*, M. M. Abbot, H. C. van Ness. McGraw-Hill, 1990.
- j. *Ejercicios de ciencias físicas: Termodinámica*, R. Annequin y J. Boutigny. Ed. Reverté, 1979.